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FOURTH-ORDER ELASTIC COEFFICIENTS FOR SOME CRYSTAL CLASSES*†

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ABSTRACT. The fourth-order elastic coefficients form an eight-order tensor containing 6561 components of which 126 are independent for a triclinic system. Using symmetry arguments it is shown that there are 70, 42, 25, and 11 independent constants for monoclinic (2, 2/m, m), orthorhombic (222, 2mm, mmm), tetragonal (4mm, $\bar{4}$2m, 422, 4/mmm) and cubic ($\bar{4}$3m, 432, m3m) crystals respectively.

INTRODUCTION

In the classical theory of elasticity the strains are treated as infinitesimal and the elastic energy of a body initially under no stresses, is a quadratic function of the strain. The stress-strain relationships and the scheme of the second-order elastic coefficients are quite well known (Huntington, 1958). In those cases where the strains may not be considered as infinitesimal, it is necessary to include higher order terms. An elegant treatment of the finite deformation of an elastic solid has been given by Murnaghan (1951). The elastic energy ϕ is analyzed into a sum

$$\phi = \phi_2 + \phi_3 + \phi_4 + \cdots$$

of terms of different degrees in the elements of η. The η's are the symmetrized Lagrangian strain components (Birch, 1947). It is possible to express ϕ_2 and ϕ_3 as

$$\phi_2 = 1/2C_{ijkl}\eta_{ij}\eta_{kl}$$
$$\phi_3 = C_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn}$$

where i, j, k, l, m, n take the values 1, 2, 3. Repeated indices imply the usual summation convention. The coefficient 1/2 in the expression for ϕ_2 is conventional. The expression for ϕ_3 follows that given by Hearmon (1953). Here the C_{ijklmn}

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†After this article was prepared, it was brought to the attention of the author of a recent communication by Krishnamurty (1963) on fourth-order elastic coefficients in crystals. For the crystal classes considered in this article, the results agree with those given by Krishnamurty.

are the third order elastic coefficients which are the components of a sixth-order tensor. Group theory has been used to determine the number of independent components of the sixth-order tensor (Bhagavantam and Suryanarayan, 1947, 1949; Jahn, 1949). Fumi (1951, 1952, 1953) has carried out an extensive investigation on "Matter Tensors" up to the sixth-order, and has given the relations between the actual components. The scheme of the third-order elastic coefficients given by Hearmon (1953, 1956) agrees with those given by Birch (1947) for cubic crystals and by Bhagavantam and Suryanarayan (1947, 1949), Jahn (1949), and Fumi (1951, 1952, 1953) for other crystal classes. The sixth-order tensor with 729 components gives only 56 independent third-order elastic coefficients for a triclinic system. This number is reduced considerably for crystals with higher symmetry. Recently, these considerations have been extended to investigate the fourth-order elastic coefficients (Ghate, 1964). In the present article, the fourth-order elastic coefficients for some crystal classes, using symmetry arguments, are enumerated.

ELASTIC ENERGY φ_4 AND THE FOURTH-ORDER ELASTIC COEFFICIENTS

Let us express ϕ_4 as follows :

$$\phi_4 = C_{ijklmnop}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op}$$

where i, j, k, l, m, n, o, p take the values 1, 2, 3. The η's are the Lagrangian strain components and the $C_{ijklmnop}$'s are the fourth-order elastic coefficients which are the components of an eighth-order tensor containing 6561 components. However, the tensor is symmetrical with respect to the interchange of i and j, k and l, ij with kl, and so on. The number of independent tensor components then reduce to 126. The components of the elastic coefficients are conventionally contracted as follows :

11—1	22—2	33—3
23—4	31—5	12—6

then $\phi_4 = C_{pqrs}\eta_p\eta_q\eta_r\eta_s$ where p, q, r, s take the values 1, 2, 3, 4, 5, 6 and C_{pqrs} are the fourth-order elastic coefficients. For a triclinic system, there are in all 126 fourth-order elastic coefficients. These are listed in Column I of Table I. Here C_{1111}, C_{1112}, etc. are written as 1111, 1112, and so on for convenience.

The contraction of the indices of $C_{ijklmnop}$ to give C_{pqrs} needs a little explanation. It may be recalled that

$$C_{pqrs} = C_{qprs} = C_{pqsr} = C_{psqr}, \text{ etc.}$$

It is convenient to define a ratio R such that

$$R \quad \frac{C_{pqrs}}{C_{ijklmnop}}$$

which gives the possible number of combinations of the indices. This point can be illustrated as follows :

$$C_{1112} = C_{11\,11\,11\,22}$$

Because of the symmetry with respect to the interchange of the indices, we have

$$C_{11\,11\,11\,22} = C_{11\,11\,22\,11} = C_{11\,22\,11\,11} = C_{22\,11\,11\,11}$$

$$\therefore\quad R = \frac{C_{1112}}{C_{11\,11\,11\,22}} = 4.$$

Similarly it can be verified that

$$C_{1122} = 6C_{11\,11\,22\,22}.$$

The values of R for all the 126 fourth-order elastic coefficients are listed in column "R" of Table I. The sum of all the values of "R" is 6561, as it should be.

TABLE I

Hermann-Mauguin symbols of the crystal classes are used at the top of each column

	Triclinic		Monoclinic		Ortho-rhombic	Tetragonal	Cubic
	1		2		222	4mm	43m
	1		2/m		-- --	42m	432
			m			422	m3m
					mmm	4/mmm	
		Mirror plane = x_2x_3 Twofold axis = x_1	Mirror plane = x_3x_1 Twofold axis x_2	Mirror plane = x_1x_2 Twofold axis = x_3			
	(126)	(70)	(70)	(70)	(42)	(25)	(11)
R	I	II	III	IV	V	VI	VII
1	1111	1111	1111	1111	1111	1111	1111
4	1112	1112	1112	1112	1112	1112	1112
4	1113	1113	1113	1113	1113	1113	1112
8	1114	1114	0	0	0	0	0
8	1115	0	1115	0	0	0	0
8	1116	0	0	1116	0	0	0
6	1122	1122	1122	1122	1122	1122	1122
12	1123	1123	1123	1123	1123	1123	1123
24	1124	1124	0	0	0	0	0
24	1125	0	1125	0	0	0	0
24	1126	0	0	1126	0	0	0
6	1133	1133	1133	1133	1133	1133	1122
24	1134	1134	0	0	0	0	0
24	1135	0	1135	0	0	0	0
24	1136	0	0	1136	0	0	0
24	1144	1144	1144	1144	1144	1144	1144
48	1145	0	0	1145	0	0	0
48	1146	0	1146	0	0	0	0

TABLE I (contd.

R	I	II	III	IV	V	VI	VII
24	1155	1155	1155	1155	1155	1155	1155
48	1156	1156	0	0	0	0	0
24	1166	1166	1166	1166	1166	1166	1155
4	1222	1222	1222	1222	1222	1112	1112
12	1223	1223	1223	1223	1223	1123	1123
24	1224	1224	0	0	0	0	0
24	1225	0	1225	0	0	0	0
24	1226	0	0	1226	0	0	0
12	1233	1233	1233	1233	1233	1233	1123
48	1234	1234	0	0	0	0	0
48	1235	0	1235	0	0	0	0
48	1236	0	0	1236	0	0	0
48	1244	1244	1244	1244	1244	1244	1244
96	1245	0	0	1245	0	0	0
96	1246	0	1246	0	0	0	0
48	1255	1255	1255	1255	1255	1244	1244
96	1256	1256	0	0	0	0	0
48	1266	1266	1266	1266	1266	1266	1266
4	1333	1333	1333	1333	1333	1333	1112
24	1334	1334	0	0	0	0	0
24	1335	0	1335	0	0	0	0
24	1336	0	0	1336	0	0	0
48	1344	1344	1344	1344	1344	1344	1244
96	1345	0	0	1345	0	0	0
96	1345	0	1346	0	0	0	0
48	1355	1355	1355	1355	1355	1355	1266
96	1356	1356	0	0	0	0	0
48	1366	1366	1366	1366	1366	1366	1244
32	1444	1444	0	0	0	0	0
96	1445	0	1445	0	0	0	0
96	1446	0	0	1446	0	0	0
96	1455	1455	0	0	0	0	0
192	1456	1456	1456	1456	1456	1456	1456
96	1466	1466	0	0	0	0	0
32	1555	0	1555	0	0	0	0
96	1556	0	0	1556	0	0	0
96	1566	0	1566	0	0	0	0
32	1666	0	0	1666	0	0	0
1	2222	2222	2222	2222	2222	1111	1111
4	2223	2223	2223	2223	2223	1113	1112
8	2224	2224	0	0	0	0	0
8	2225	0	2225	0	0	0	0
8	2226	0	0	2226	0	0	0
6	2233	2233	2233	2233	2233	1133	1122
24	2234	2234	0	0	0	0	0

TABLE I—(contd.)

R	I	II	III	IV	V	VI	VII
24	2235	0	2235	0	0	0	0
24	2236	0	0	2236	0	0	0
24	2244	2244	2244	2244	2244	1155	1155
48	2245	0	0	2245	0	0	0
48	2246	0	2246	0	0	0	0
24	2255	2255	2255	2255	2255	1144	1144
48	2256	2256	0	0	0	0	0
24	2266	2266	2266	2266	2266	1166	1155
4	2333	2333	2333	2333	2333	1333	1112
24	2334	2334	0	0	0	0	0
24	2335	0	2335	0	0	0	0
24	2336	0	0	2336	0	0	0
48	2344	2344	2344	2344	2344	1355	1266
96	2345	0	0	2345	0	0	0
96	2346	0	2346	0	0	0	0
48	2355	2355	2355	2355	2355	1344	1244
96	2356	2356	0	0	0	0	0
48	2366	2366	2366	2366	2366	1366	1244
32	2444	2444	0	0	0	0	0
96	2445	0	2445	0	0	0	0
96	2446	0	0	2446	0	0	0
96	2455	2455	0	0	0	0	0
192	2456	2456	2456	2456	2456	1456	1456
96	2466	2466	0	0	0	0	0
32	2555	0	2555	0	0	0	0
96	2556	0	0	2556	0	0	0
96	2566	0	2566	0	0	0	0
32	2666	0	0	2666	0	0	0
1	3333	3333	3333	3333	3333	3333	1111
8	3334	3334	0	0	0	0	0
8	3335	0	3335	0	0	0	0
8	3336	0	0	3336	0	0	0
24	3344	3344	3344	3344	3344	3344	1155
48	3345	0	0	3345	0	0	0
48	3346	0	3346	0	0	0	0
24	3355	3355	3355	3355	3355	3344	1155
48	3356	3356	0	0	0	0	0
24	3366	3366	3366	3366	3366	3366	1144
32	3444	3444	0	0	0	0	0
96	3445	0	3445	0	0	0	0
96	3446	0	0	3446	0	0	0
96	3455	3455	0	0	0	0	0
192	3456	3456	3456	3456	3456	3456	1456
96	3466	3466	0	0	0	0	0
32	3555	0	3555	0	0	0	0

TABLE I (contd.)

R	I	II	III	IV	V	VI	VII
96	3556	0	0	3556	0	0	0
96	3566	0	3566	0	0	0	0
32	3666	0	0	3666	0	0	0
16	4444	4444	4444	4444	4444	4444	4444
64	4445	0	0	4445	0	0	0
64	4446	0	4446	0	0	0	0
96	4455	4455	4455	4455	4455	4455	4455
192	4456	4456	0	0	0	0	0
96	4466	4466	4466	4466	4466	4466	4455
64	4555	0	0	4555	0	0	0
192	4556	0	4556	0	0	0	0
192	4566	0	0	4566	0	0	0
64	4666	0	4666	0	0	0	0
16	5555	5555	5555	5555	5555	4444	4444
64	5556	5556	0	0	0	0	0
96	5566	5566	5566	5566	5566	4466	4455
64	5666	5666	0	0	0	0	0
16	6666	6666	6666	6666	6666	6666	4444

Finally we note that the n-th order elastic coefficients form a $2n$-order-tensor with 3^{2n} components. It is easy to convince oneself that the number of independent coefficients is given by

$$\frac{6.(6+1)\ldots(6+n-1)}{n!}$$

FOURTH-ORDER ELASTIC COEFFICIENTS FOR SOME CRYSTAL CLASSES

If the crystal possesses certain symmetry properties, then the elastic energy should be invariant with respect to these symmetry operations. In the following discussion, the primed axes will imply the new set of axes obtained after a symmetry operation.

Monoclinic Crystals (2, $2/m.m$) : We take a coordinate system with x_2x_3 as the plane of symmetry. On reflection in this plane, we obtain the new set of axes.

$$x_1' = -x_1;\ x_2' = x_2;\ x_3' = x_3.$$

The primed and the unprimed strain components are related to each other in the following manner :

$$\eta_1' = \eta_1,\ \eta_2' = \eta_2,\ \eta_3' = \eta_3;\ \eta_4' = \eta_4,\ \eta_5' = -\eta_5,\ \eta_6' = -\eta_6.$$

The elastic energy should be invariant with respect to this operation and therefore

$$\phi_4 = C_{pqrs}\eta_p\eta_q\eta_r\eta_s = C_{ijkl}\eta_i'\eta_j'\eta_k'\eta_l$$

where p, q, r, s, i, j, k, l take the values 1, 2, 3, 4, 5, 6. It follows that :

$$C_{1113}\eta_1^3 \eta_5 = -C_{1113}\eta_1^3 \eta_5; \quad \therefore \quad C_{1115} = 0.$$

All the nonvanishing coefficients can be found in a similar manner. These are listed in column II of Table I. In all there are 70 independent fourth-order elastic coefficients. In columns III and IV, the coefficients are listed for those cases where x_3x_1 and x_1x_2 are the planes of symmetry.

Orthorhombic Crystals (222, 2*mm* *mmm*) : Take the three planes of symmetry as the coordinate planes. It can be easily verified that only those coefficients which are common to columns 2, 3 and 4 are the required ones. Thus we find that there are only 42 independent fourth-order elastic coefficients for an orthorhombic system. These are listed in column V of Table I.

Tetragonal Crystals (4*mm*, $\bar{4}2m$, 422, 4/*mmm*): In the case of the tetragonal crystals there is a four-fold axis in addition to the three planes of symmetry, which are taken as the coordinate planes. The "x_3" axis is chosen as the four-fold axis. It is evident that we have to examine the 42 coefficients of the orthorhombic system for further interrelationships. For a rotation of $\pi/2$ about the "x_3" axis, the primed and the unprimed strain components are related to each other as follows :

$$\eta_1' = \eta_2, \eta_2' = \eta_1, \eta_3' = \eta_3; \eta_4' = -\eta_5, \eta_5' = \eta_4, \eta_6' = -\eta_6.$$

The elastic energy ϕ_4 must be insensitive to this covering operation. The following relations are then obtained :

$$1111 = 2222; \quad 1112 = 1222; \quad 1113 = 2223; \quad \text{and so on.}$$

There are in all 25 independent coefficients which are listed in column VI of Table I. The other equivalent coefficients, for example, 1456 = 2456, can be easily obtained from Table I.

Cubic Crystals (43*m*, 432, *m*3*m*) : Take the cartesian coordinate axes (x_1, x_2, x_3) as coinciding with a set of cubic axes. Note that each cubic axis is a four-fold axis and hence has the tetragonal symmetry. Thus it is necessary to examine only the independent coefficients of the tetragonal system for additional interrelationships. It is further noted that each body diagonal is a three-fold axis. A rotation of $2\pi/3$ about the body diagonal defines a new set of axis such that x_1' coincides with x_2, x_2' coincides with x_3, and x_3' coincides with x_1. The primed and the unprimed strain components are related to each other in the following manner :

$$\eta_1' = \eta_2, \eta_2' = \eta_3, \eta_3' = \eta_1; \eta_4' = \eta_5, \eta_5' = \eta_6, \eta_6' = \eta_4.$$

The elastic energy ϕ_4 has to be invariant for these symmetry operations. It is found that,

$$1111 = 2222 = 3333$$

$$1112 = 1113 = 1222 = 1333 = 2223 = 2333$$

and so on. There are in all 11 independent coefficients for a cubic crystal and these are listed in column VII of Table I.

Elastic Energy ϕ_4

The use of the table in writing the terms of the elastic energy ϕ_4 for a cubic crystal will now be illustrated. For a particular constant, say 1244, scan the column VII downwards and find out how many times it appears. Every time 1244 is found, look for the corresponding coefficient in the column for the triclinic system. Note that, $1244 = 2366 = 1344 = 1366 = 2355 = 1255$. That part of the elastic energy with coefficient C_{1244}, can now be written as

$$C_{1244}(\eta_1\eta_2(\eta_4^2+\eta_5^2)+\eta_2\eta_3(\eta_5^2+\eta_6^2)+\eta_1\eta_3(\eta_6^2+\eta_4^2)).$$

The total elastic energy ϕ_4 can now be easily written as follows :

$$\begin{aligned}
\phi_4 = {} & C_{1111}(\eta_1^4+\eta_2^4+\eta_3^4) \\
& +C_{1112}(\eta_1^3(\eta_2+\eta_3)+\eta_2^3(\eta_3+\eta_1)+\eta_3^3(\eta_1+\eta_2)) \\
& +C_{1122}(\eta_1^2\eta_2^2+\eta_2^2\eta_3^2+\eta_3^3\eta_1^2) \\
& +C_{1123}(\eta_1^2\eta_2\eta_3+\eta_2^2\eta_3\eta_1+\eta_3^2\eta_1\eta_2) \\
& +C_{1144}(\eta_1^2\eta_4^2+\eta_2^2\eta_5^2+\eta_3^2\eta_6^2) \\
& +C_{1155}(\eta_1^2(\eta_5^2+\eta_6^2)\eta_2^2(\eta_4^2+\eta_6^2)\eta_3^2(\eta_4^2+\eta_5^2)) \\
& +C_{1244}(\eta_1\eta_2(\eta_4^2+\eta_5^2)+\eta_2\eta_3(\eta_5^2+\eta_6^2)+\eta_1\eta_3(\eta_6^2+\eta_4^2)) \\
& +C_{1266}(\eta_1\eta_2\eta_6^2+\eta_2\eta_3\eta_4^2+\eta_3\eta_1\eta_5^2) \\
& +C_{1456}(\eta_4\eta_5\eta_6(\eta_1+\eta_2+\eta_3)) \\
& +C_{4444}(\eta_4^4+\eta_5^4+\eta_6^4) \\
& +C_{4455}(\eta_4^2\eta_5^2+\eta_5^2\eta_6^2+\eta_6^2\eta_4^2).
\end{aligned}$$

Table I can be used to write ϕ_4 for other crystal classes. It may be remarked, however, that the independent fourth-order elastic coefficients for the hexagonal and trigonal systems can be deduced, starting from the 70 independent coefficients of the monoclinic system, except for the formidable algebra involved.

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